

# Erratum

## SHAKE, Rattle, and Roll: Efficient Constraint Algorithms for Linked Rigid Bodies

**TIMOTHY R. FORESTER, WILLIAM SMITH**

*Department for Computation and Information, CCLRC Daresbury Laboratory, Daresbury, Warrington, Cheshire WA4 4AD, United Kingdom*

*Volume 19, Number 1, pages 102–111, 1998*

There is an error of omission of the centrifugal terms from the description of the angular motion, which spans eqs. (6) to (11). The simplest fix appears to be to rewrite eq. (7) in the following manner:

$$\hat{\underline{\tau}} = \underline{\underline{R}} \cdot \underline{\underline{\tau}} + \underline{\eta} \quad (7a)$$

$$\eta_x = (\hat{\underline{I}}_{yy} - \hat{\underline{I}}_{zz})\hat{\omega}_y\hat{\omega}_z \quad (\text{etc.}) \quad (7b)$$

where (7b) implies cyclic permutations of  $x$ ,  $y$ , and  $z$ . This redefinition corrects all the subsequent equations.

This amendment has no impact on the description of the main subject of the paper (the QSHAKE algorithm) and the eqs. (20) to (29) are unaffected. Though the reader may think that eq. (22) requires a similar amendment, this is not the case, as the QSHAKE algorithm represents a perturbative correction to the normal equations of motion, which (should!) already contain the centrifugal contributions.